Sulfaguanidine

57-67-0 | DTXSID1023609

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 258 °C

Global applicability domain: Outside

Local applicability domain index: 9.80e-02

Confidence level: 7.45e-01

Nearest Neighbors from the Training Set

N-(4-Bromophenyl)urea
Measured: 260
Predicted: 256

1-Phenylurea
Measured: 238
Predicted: 247

Diphenylurea
Measured: 262
Predicted: 269

N,N'-Dimethylurea
Measured: 269
Predicted: 267

Urea, N,N'-diethyl (9CI)
Measured: 263
Predicted: 262